

Powder Diffraction Study of Hectorite

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Beamline(s): X7A

Smectite clays are both dioctahedral and trioctahedral layered minerals which display the interesting property of being able to expand and contract their structures along the [001] direction while maintaining two-dimensional crystallographical integrity. Expansion may take place when water or some polar organic compound enters the interlayer space. When smectite expands the interlayer cation maybe replaced and exchange takes place.[1] Due to this adaptability and their availability these minerals are being investigated for applications as electrodes, catalysis composites and electrical devices.[2] Hectorite is a trioctahedral smectite and has an ideal formula $R_{0.33}^{+}(Mg_{2.67}Li_{0.33})Si_4O_{10}(OH)_2$, where R is the exchangeable cation.

Powder diffraction data have been collected at X7A using a wavelength of 0.7 Å for two specimens of Na fluorohectorite ($Na_{0.3}(Mg_2Li)Si_4O_{10}F_2$): a flat plate and a rotating capillary. Selected regions of both diffractograms are shown in **Figure 1**. Clear differences in the intensity profiles can be observed. The basal peaks (00l) are very much enhanced in the flat plate where the material is well oriented, and nine orders are clearly observed. The differences in the peak widths observed in the spectra are mainly due to the instrument resolution since different detectors were used in the measurements (PSD and analyser, for the flat plate and capillary, respectively). The sharpest reflections are from quartz present in the samples, which illustrate the resolution differences between the analyser and the PSD.

A preliminary Williamson-Hall analysis of the first basal peaks returns the same lattice strain, $\Delta d/d = 0.5\%$, for both the oriented and non-oriented samples. The coherence length perpendicular to the [001] direction, is also similar in both cases (≈ 3000 Å) showing long-range order perpendicular to [001].

The data taken from the non-oriented material in a rotating capillary allows determination of the monoclinic unit cell parameters as $a = 5.254(1)$ Å, $b = 9.187(2)$ Å, $c = 12.506(3)$ Å, $\beta = 99.02(1)^\circ$, in agreement with those in the literature [3]. Work is in progress to study the structural changes associated with the cation exchange and expansion of these unique materials.

References: [1] D. M. Moore and R.C. Reynolds, "X-ray diffraction and the identification and analysis of clay minerals". Oxford University Press (Oxford-New York, 1997).

[2] P.D. Kaviratna, T.J. Pinnavaia, and Schroeder, "Dielectric properties of smectite clays", *J. Phys. Chem. Solids*, **57**, p.1897-1905 (1996).

[3] Encyclopedia of Minerals, 2nd Edition, 1990.

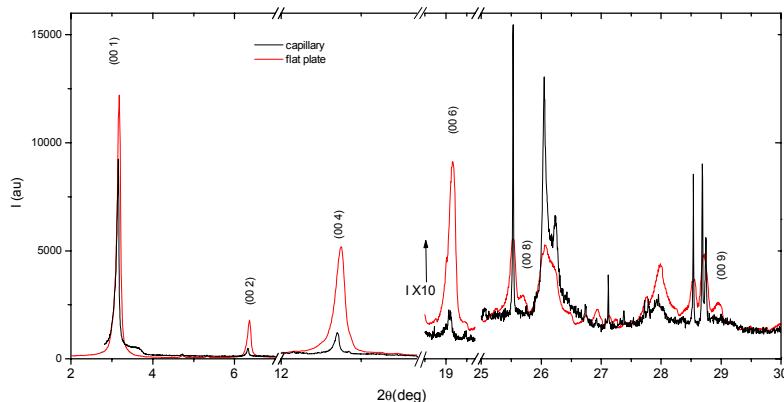


Figure 1. Powder diffraction data of Hectorite. Flat plate and capillary measurements are shown as red and black lines, respectively. The enhancement of the basal peaks in the flat plate specimen is clearly observed. Quartz peaks are also present.